User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 02/04/2002 Time: 13:43:10

Sample: AE00840
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 2/4/02 13:42 Ended: 2/4/02 13:42 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		83		5.0

Comments for Sample AE00840 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 02-04-2002 Time: 13:43:47

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds. The recoveries for 7 of the 43 compounds in the LCS Standard were above their acceptance ranges.

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 01 08:46:10 2002 Quant Results File: SCAN508.RES

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration
DataAcq Meth : SCAN508

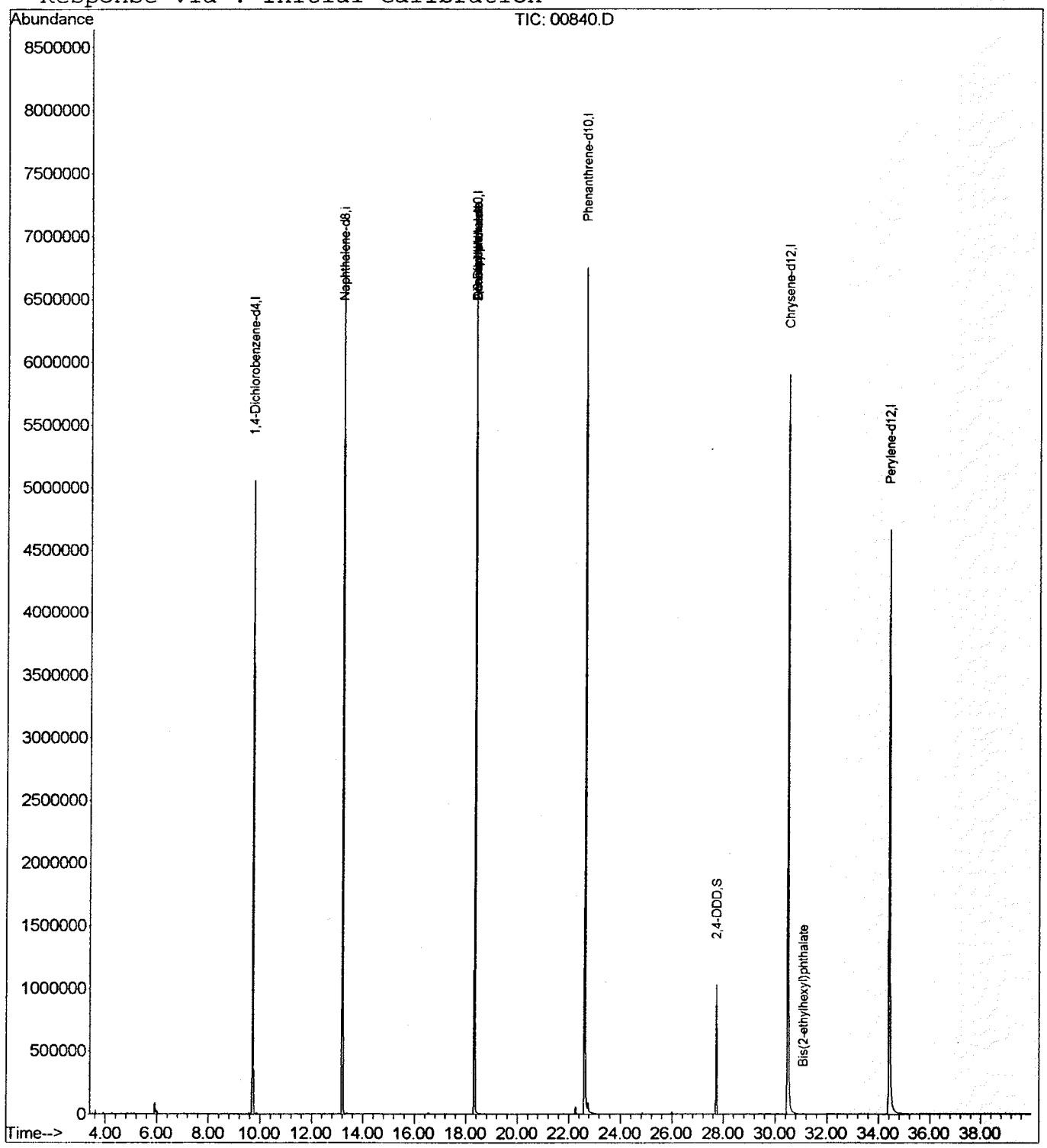
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1680051	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	7126693	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	3649679	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	5979882	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	5268792	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3797765	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	393388	4.16	ug/L	0.00
Spiked Amount 5.000			Recovery = 83.20%			
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	573741	2.38	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	456016	9.70	ug/L #	17
42) Bis(2-ethylhexyl)phthalate	31.09	149	6858	0.57	ug/L	91

(#) = qualifier out of range (m) = manual integration
00840.D SCAN508.M Fri Feb 01 08:46:12 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 1 8:46 2002 Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Smoothing : OFF Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.2 Max Peaks: 20
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

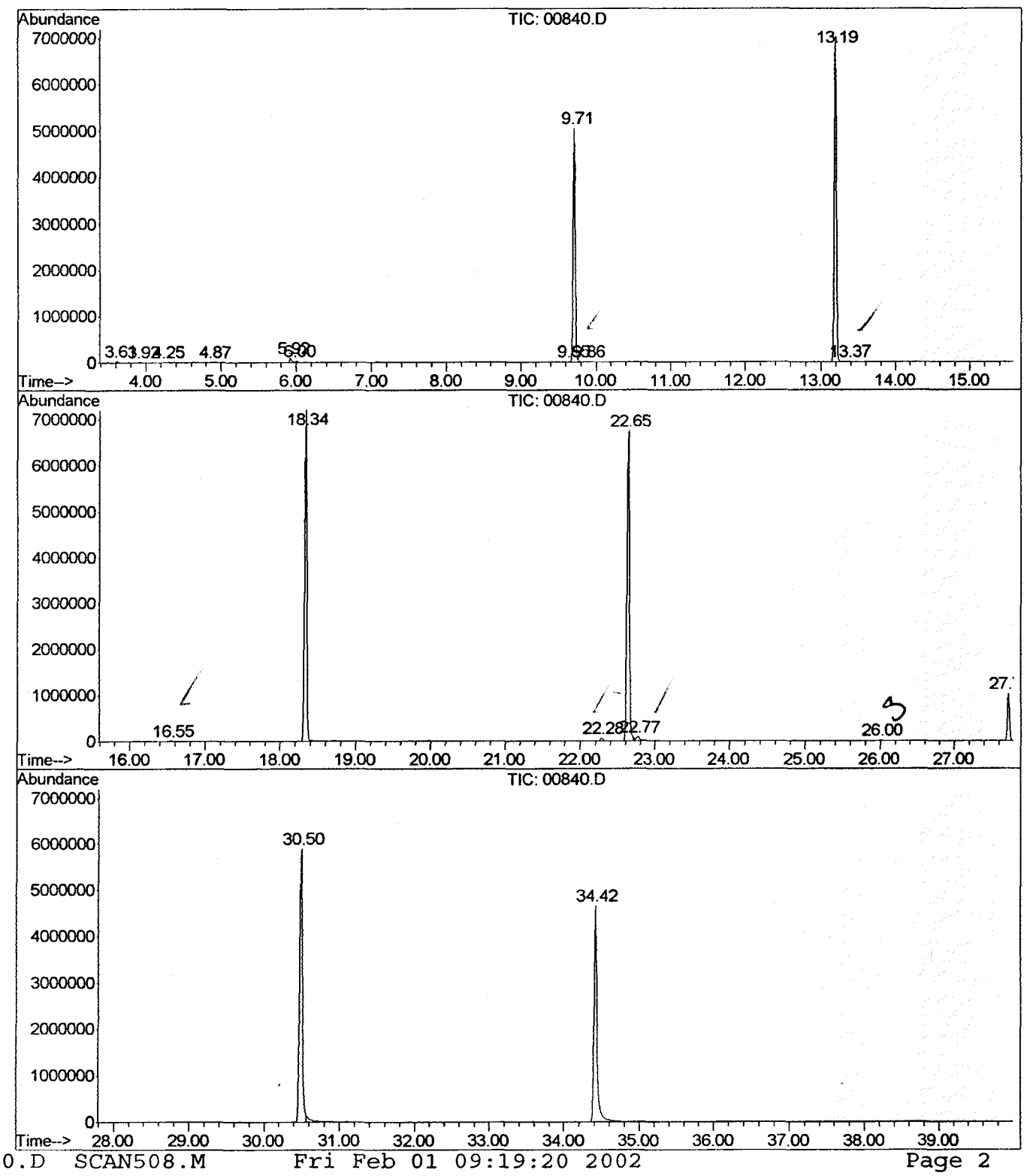
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.613	17	21	25	rBV	36119	52027	0.33%	0.061%
2	3.922	45	48	53	rBV	15294	25435	0.16%	0.030%
3	4.253	75	77	85	rVV3	12867	28414	0.18%	0.033%
4	4.869	129	131	141	rVV3	8948	33762	0.21%	0.040%
5	5.920	221	223	229	rVV	91551	190779	1.20%	0.224%
6	6.000	229	230	237	rVV	30187	57741	0.36%	0.068%
7	9.653	541	550	551	rBV2	10357	39187	0.25%	0.046%
8	9.710	551	555	561	rVV	5056442	9625839	60.66%	11.307%
9	9.858	561	568	583	rVB2	13618	60202	0.38%	0.071%
10	13.192	855	860	865	rBV	7021538	13772277	86.79%	16.178%
11	13.375	871	876	883	rVB	16684	35578	0.22%	0.042%
12	16.549	1149	1154	1159	rVB2	17590	35098	0.22%	0.041%
13	18.341	1305	1311	1315	rBV	7205289	14679664	92.51%	17.244%
14	22.280	1651	1656	1661	rBV2	63263	124660	0.79%	0.146%
15	22.645	1681	1688	1693	rVV2	6750390	15867918	100.00%	18.639%
16	22.771	1695	1699	1729	rVB	92154	416882	2.63%	0.490%
17	26.002	1979	1982	1987	rBV	20586	40579	0.26%	0.048%
18	27.726	2129	2133	2137	rBV	1028658	1903890	12.00%	2.236%
19	30.500	2369	2376	2381	rBV	5898946	15221313	95.93%	17.880%
20	34.416	2713	2719	2757	rBV	4658188	12919924	81.42%	15.176%

Sum of corrected areas: 85131169

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN31\00840.D
Operator :
Acquired : 31 Jan 2002 5:11 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 31, 2002
Vial Number: 4
Quant File :SCAN508.RES (RTE Integrator)



Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

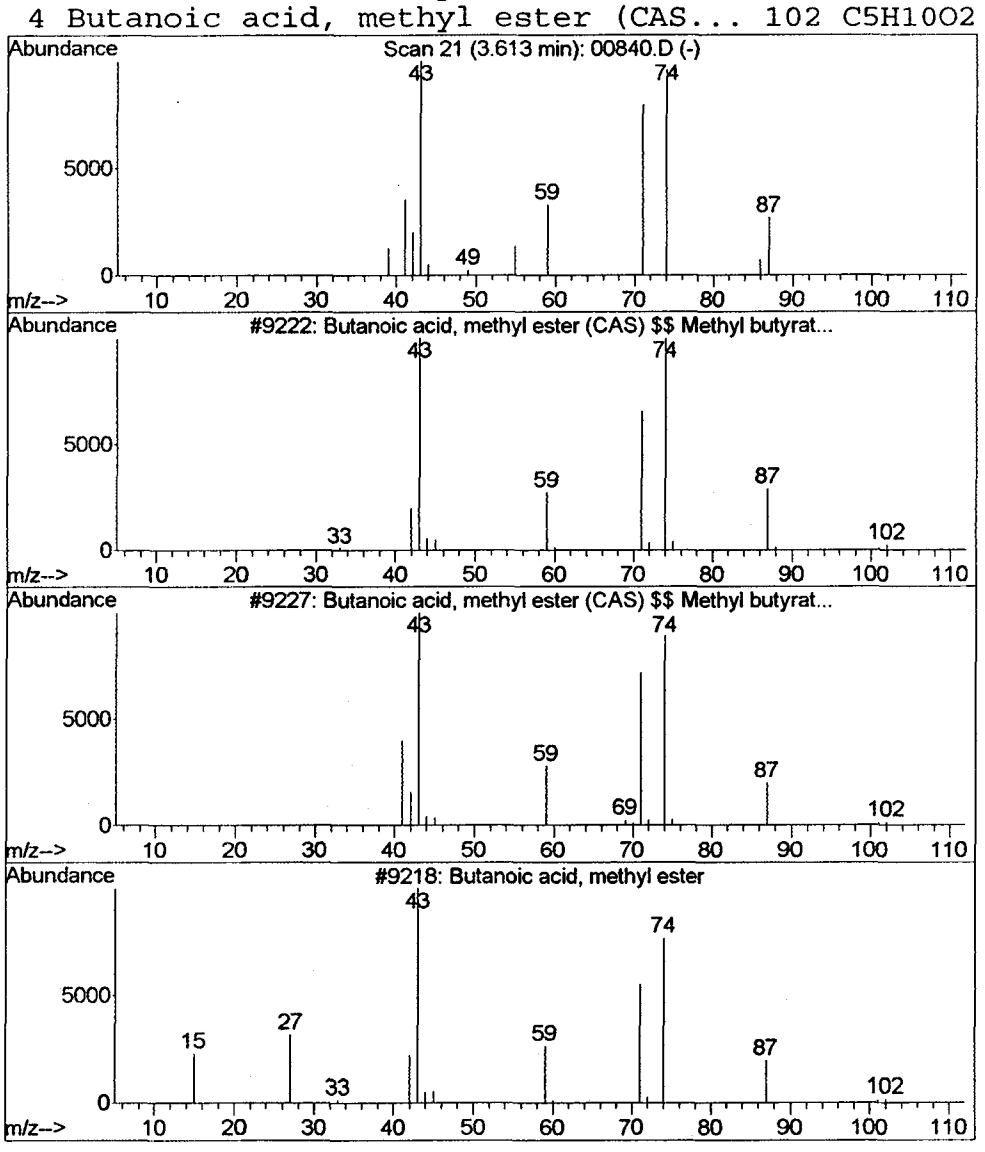
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

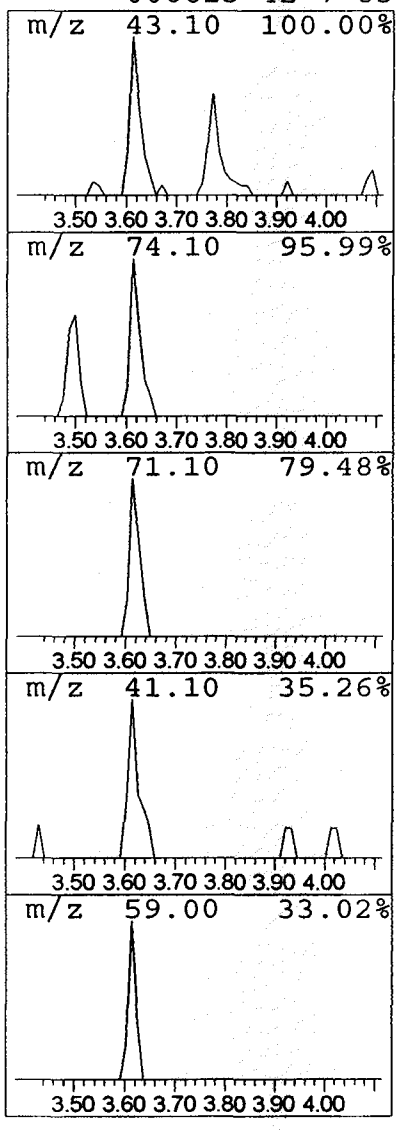
****

Peak Number 1 Butanoic acid, methyl ester... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.61	0.11 ug/L	52027	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
2	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
4	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

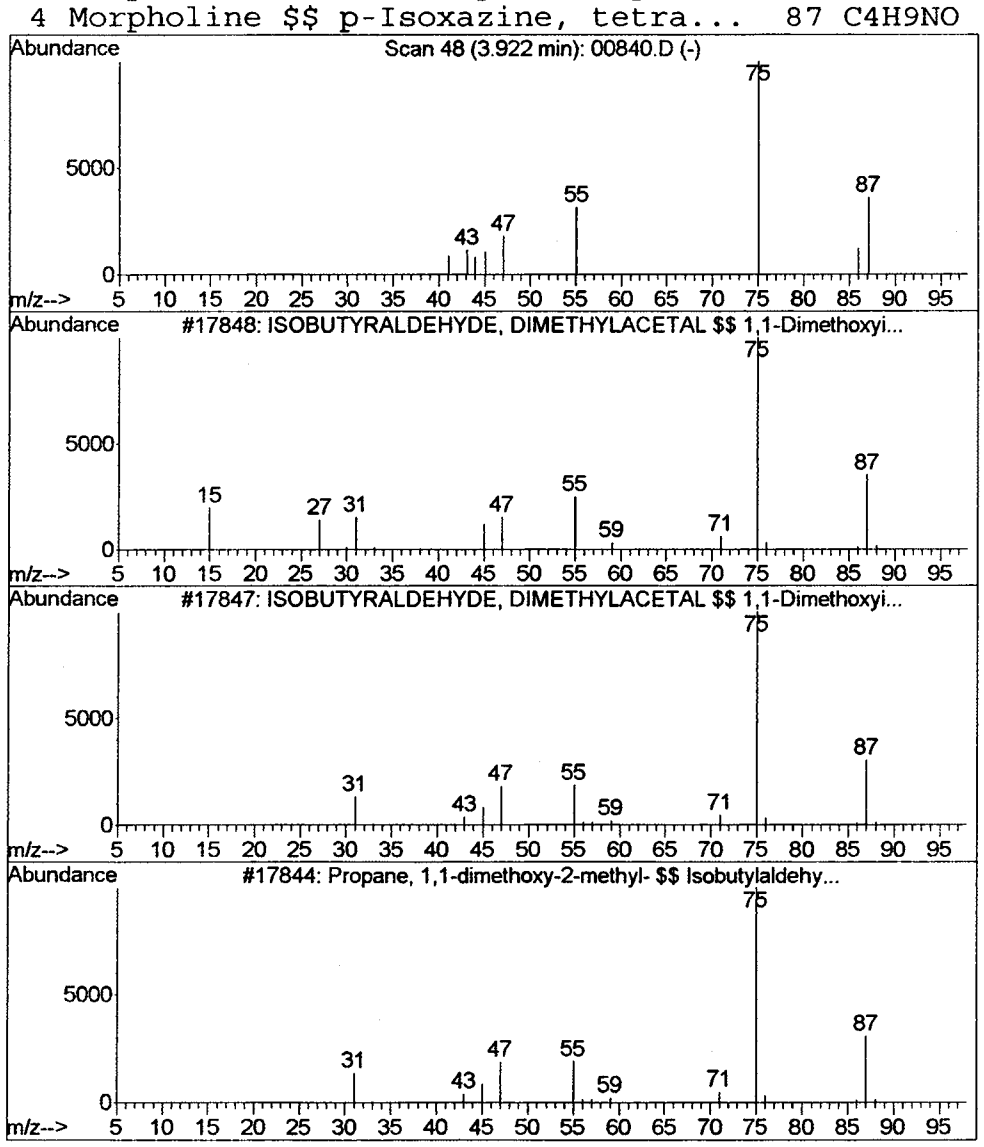
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

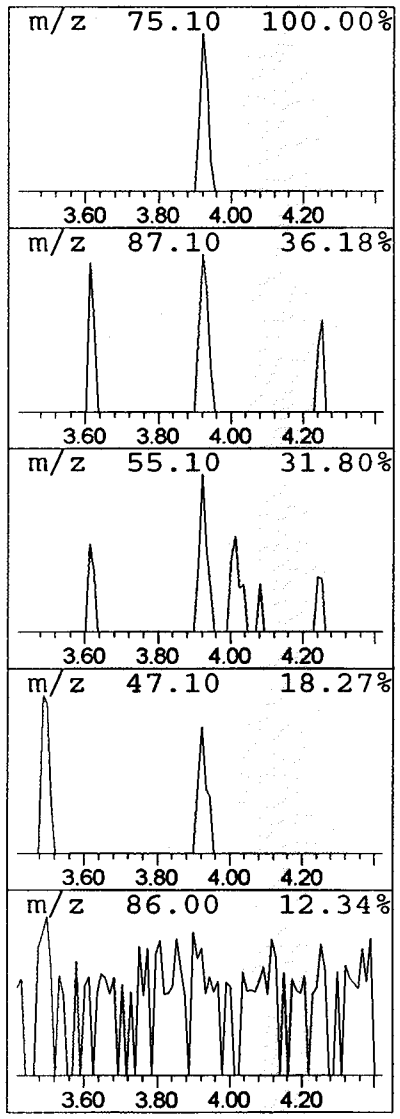
****

Peak Number 2 ISOBUTYRALDEHYDE, DIMETHYLA... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	0.05 ug/L	25435	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	ISOBUTYRALDEHYDE, DIMETHYLACETAL...	118	C6H14O2	000000-00-0	64
2	ISOBUTYRALDEHYDE, DIMETHYLACETAL...	118	C6H14O2	000000-00-0	9
3	Propane, 1,1-dimethoxy-2-methyl-...	118	C6H14O2	041632-89-7	9
4	Morpholine $$ p-Isoxazine, tetra...	87	C4H9NO	000110-91-8	4





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

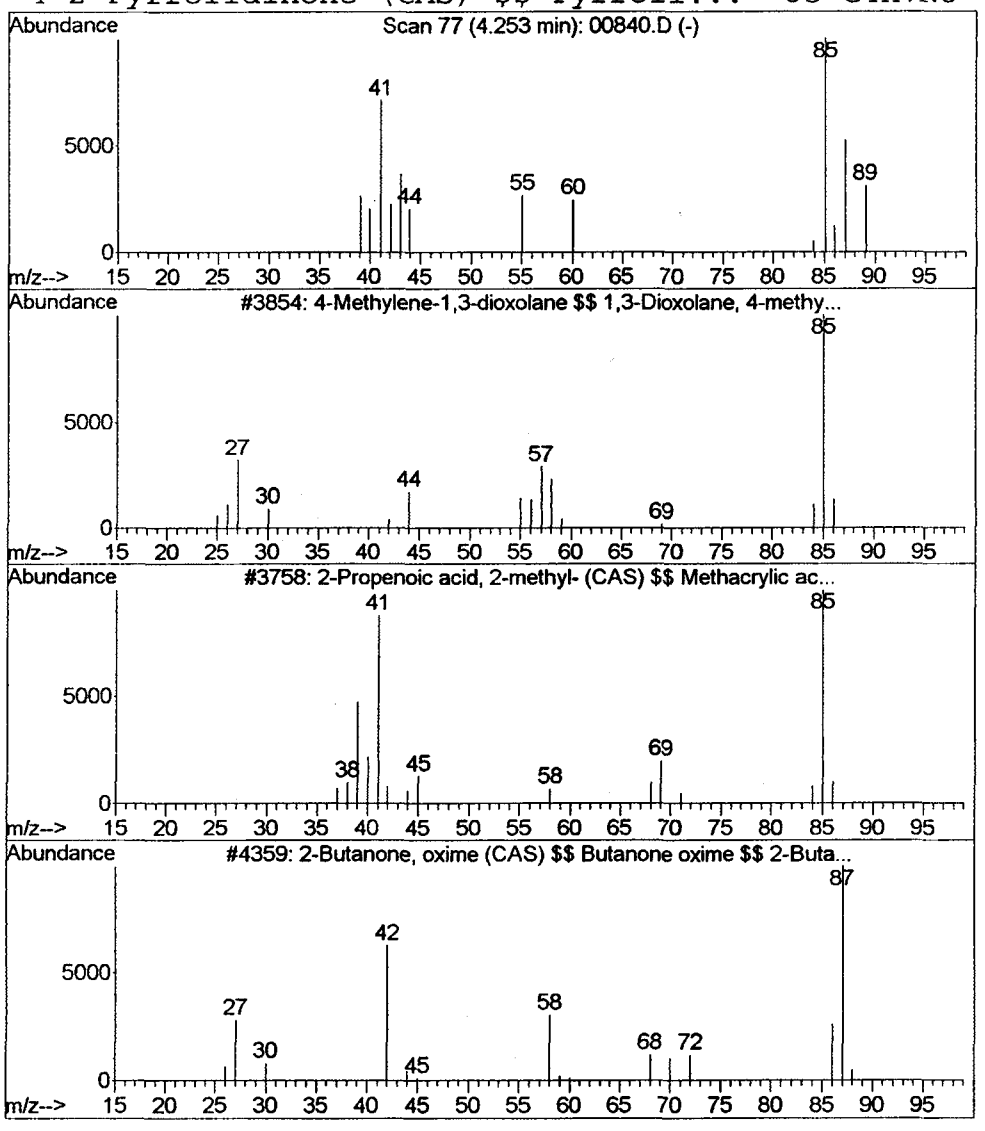
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

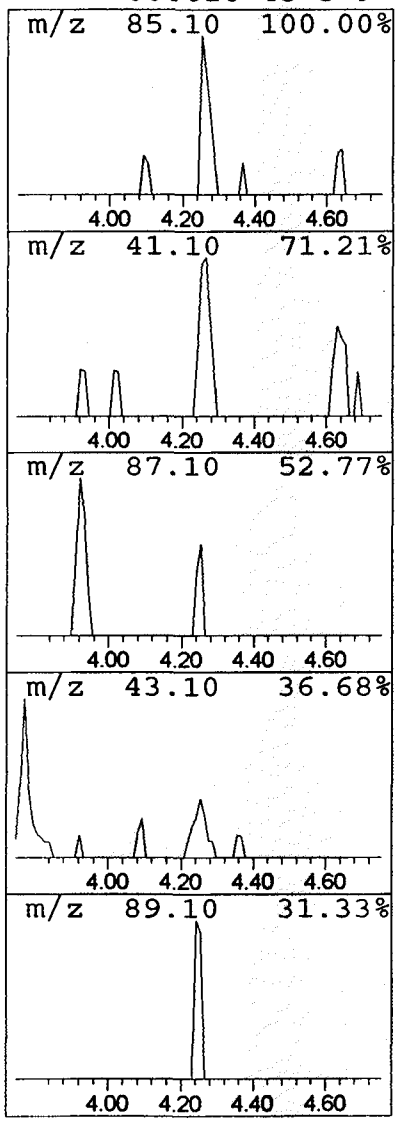
****

Peak Number 3 4-Methylene-1,3-dioxolane $... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.25	0.06 ug/L	28414	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylene-1,3-dioxolane $$ 1,3...	86	C4H6O2	004362-24-7	9
2	2-Propenoic acid, 2-methyl- (CAS...	86	C4H6O2	000079-41-4	9
3	2-Butanone, oxime (CAS) $$ Butan...	87	C4H9NO	000096-29-7	9
4	2-Pyrrolidinone (CAS) $$ Pyrroli...	85	C4H7NO	000616-45-5	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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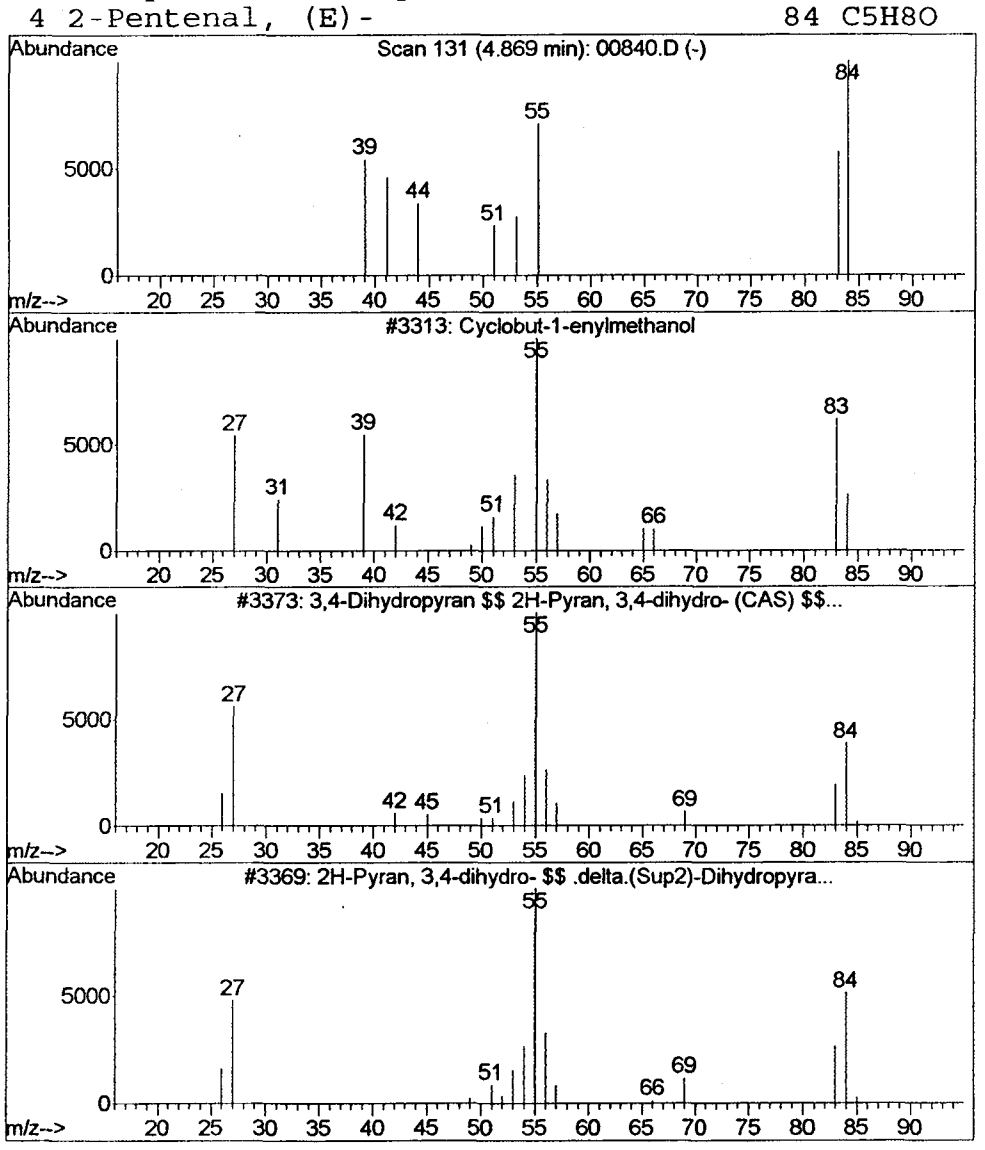
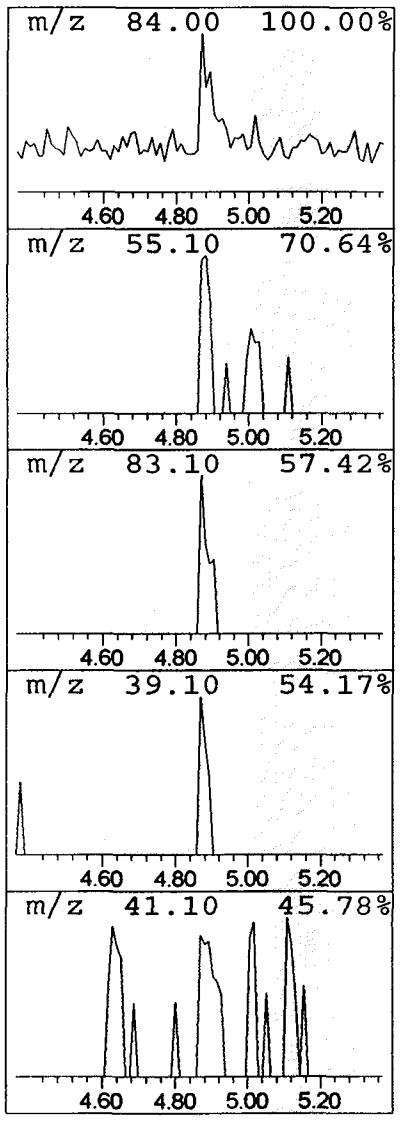
Peak Number 4 Cyclobut-1-enylmethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	0.07 ug/L	33762	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobut-1-enylmethanol	84	C5H8O	000000-00-0	9
2	3,4-Dihydropyran $$ 2H-Pyran, 3,...	84	C5H8O	000110-87-2	7
3	2H-Pyran, 3,4-dihydro- $$ .delta...	84	C5H8O	000110-87-2	7
4	2-Pentenal, (E)-	84	C5H8O	001576-87-0	7





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

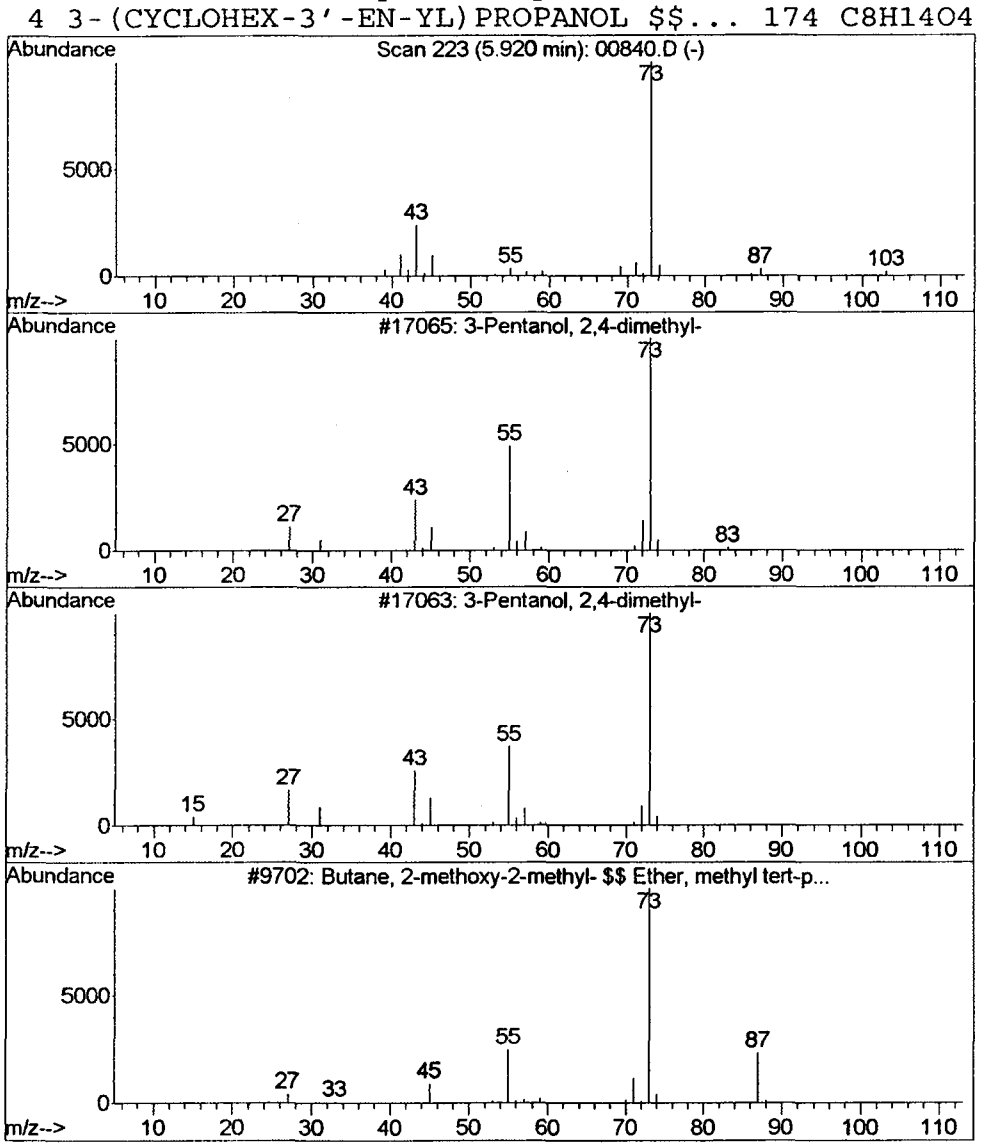
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

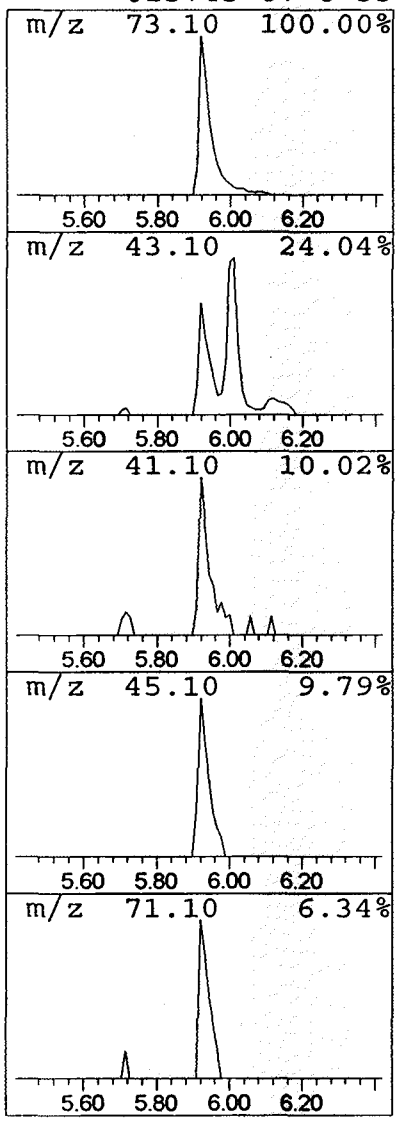
****

Peak Number 5 3-Pentanol, 2,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	0.40 ug/L	190779	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	36
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	36
3	Butane, 2-methoxy-2-methyl- $$ E...	102	C6H14O	000994-05-8	36
4	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	33





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

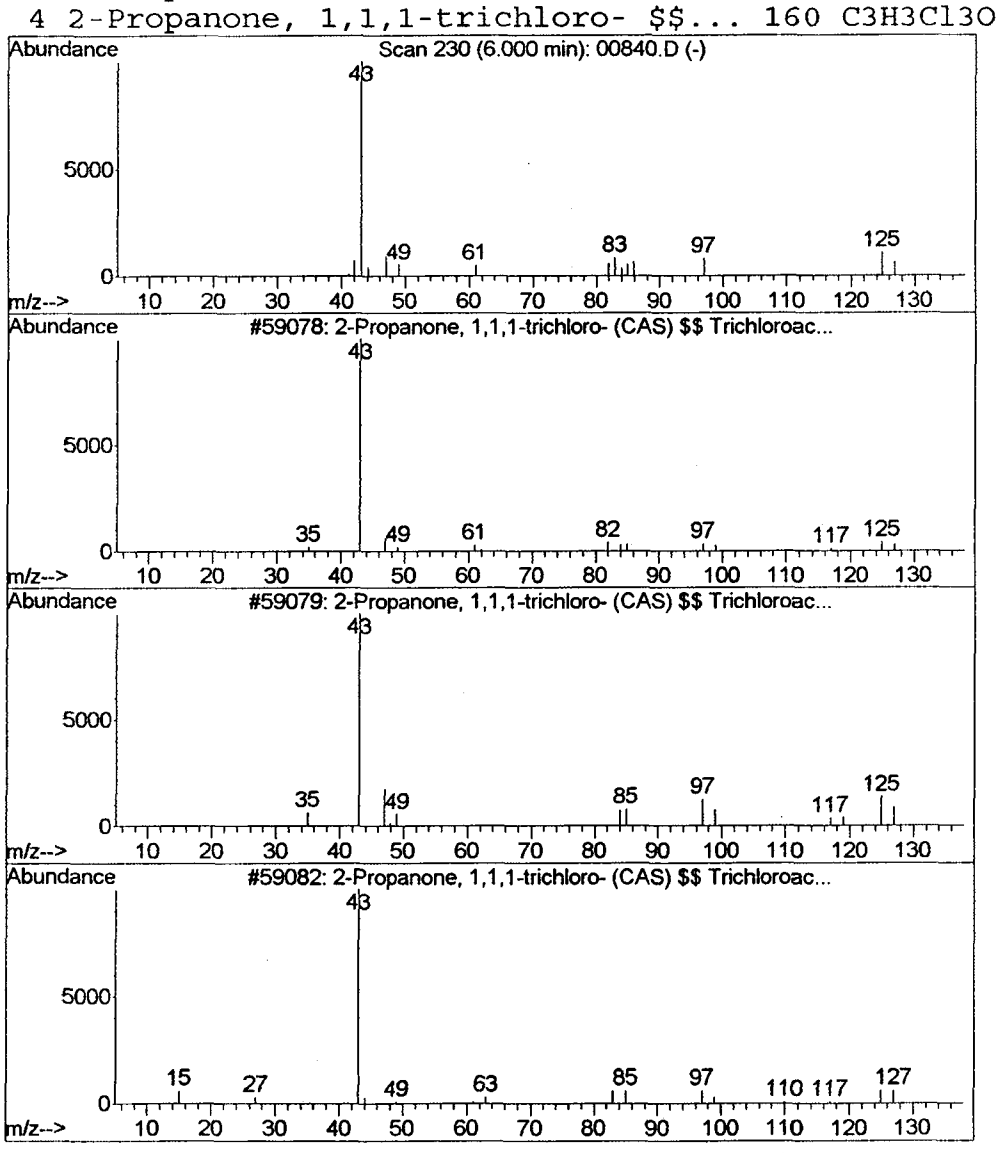
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

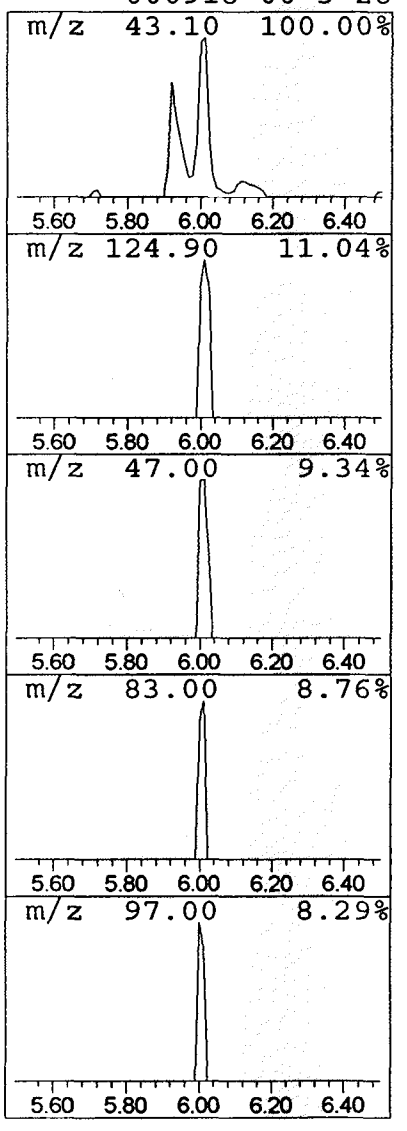
****

Peak Number 6 2-Propanone, 1,1,1-trichlor... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	0.12 ug/L	57741	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	78
2	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	53
3	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	28
4	2-Propanone, 1,1,1-trichloro- $$...	160	C3H3Cl3O	000918-00-3	28





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

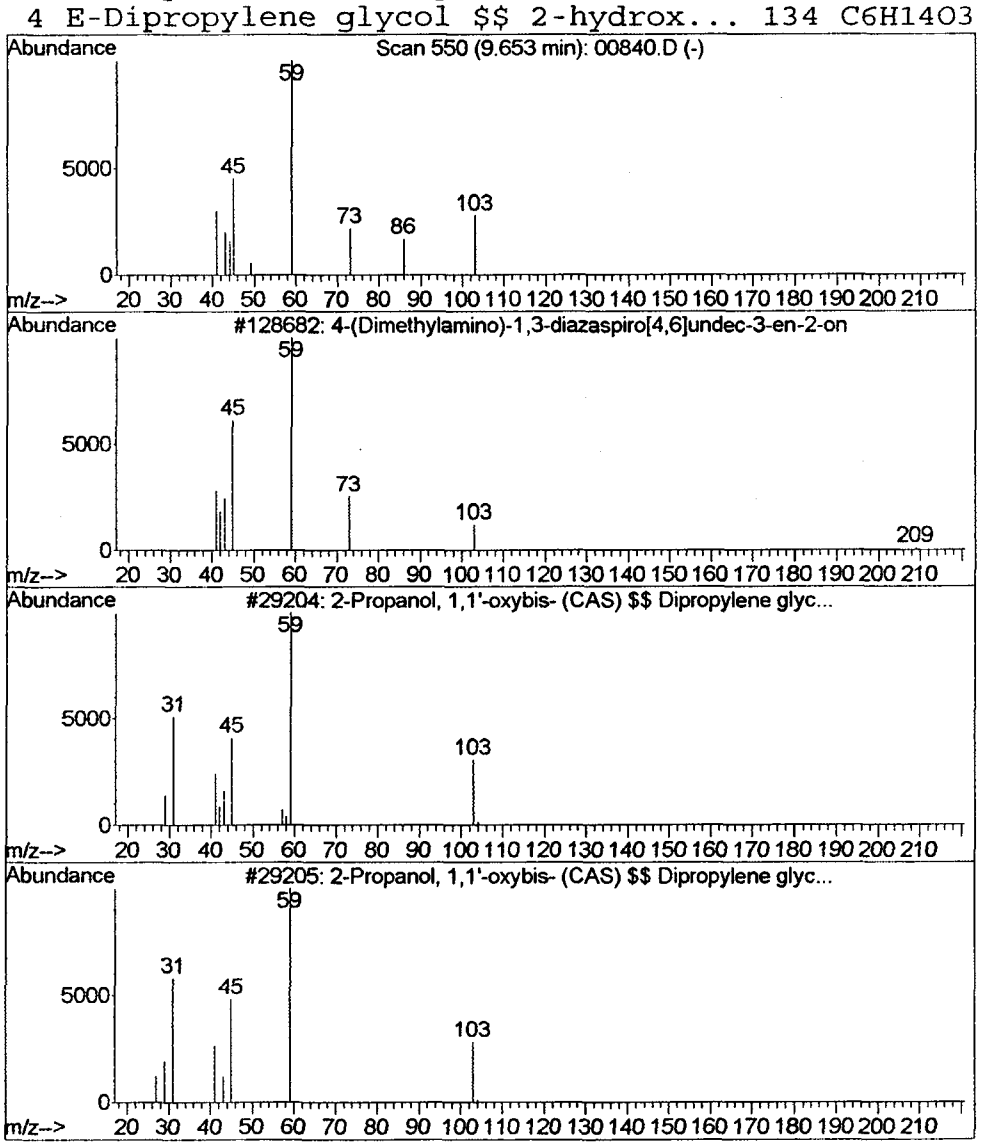
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

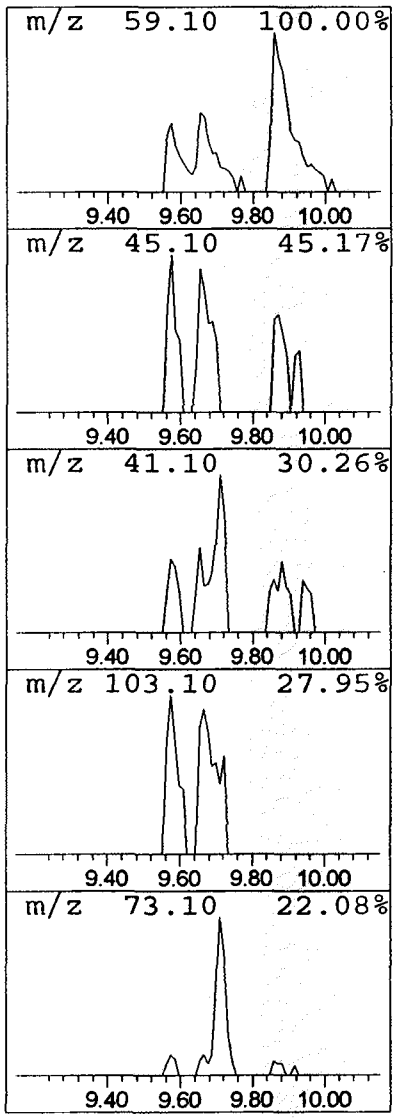
****

Peak Number 7 4-(Dimethylamino)-1,3-diaza... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	0.08 ug/L	39187	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(Dimethylamino)-1,3-diazaspiro...	209	C11H19N3O	000000-00-0	39
2	2-Propanol, 1,1'-oxybis- (CAS) $...	134	C6H14O3	000110-98-5	39
3	2-Propanol, 1,1'-oxybis- (CAS) $...	134	C6H14O3	000110-98-5	9
4	E-Dipropylene glycol $$ 2-hydrox...	134	C6H14O3	000000-00-0	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

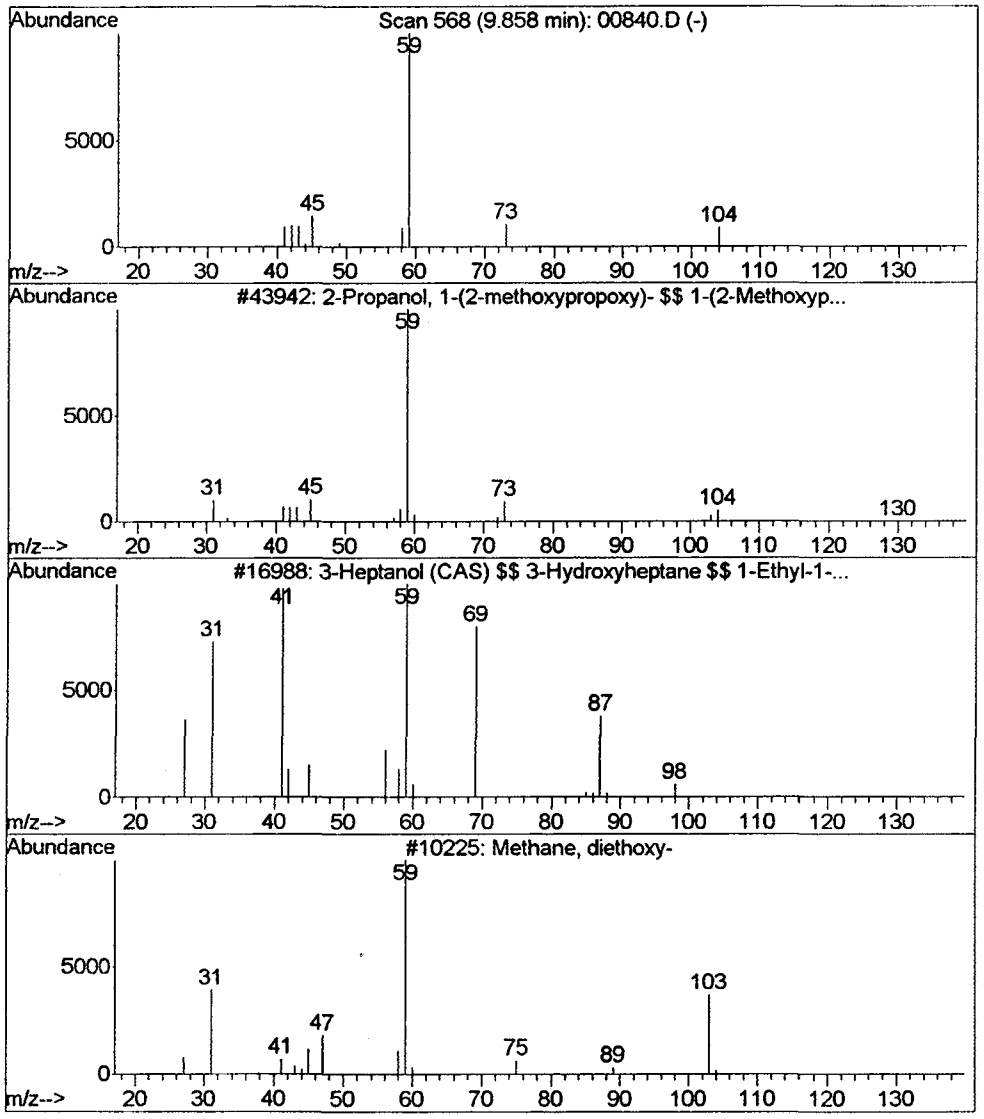
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

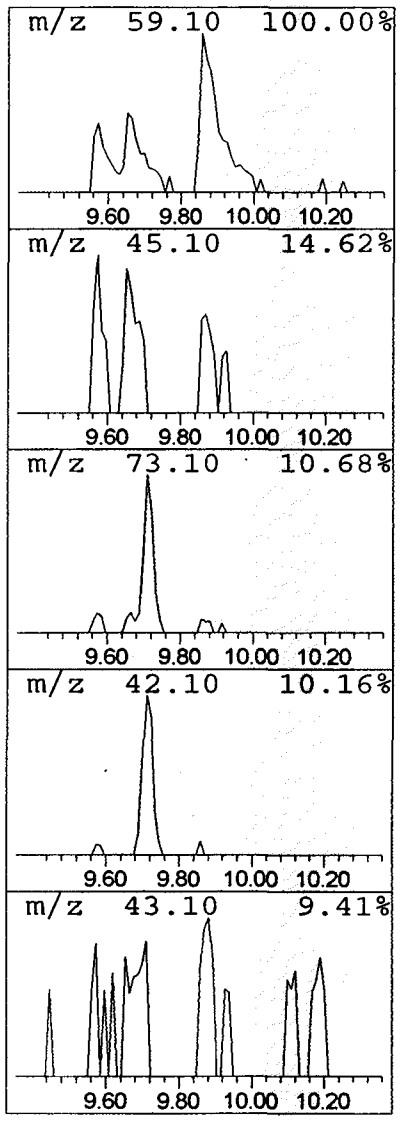
****

Peak Number 8 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.86	0.13 ug/L	60202	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)...	148	C7H16O3	013429-07-7	83
2	3-Heptanol (CAS) $$ 3-Hydroxyhep...	116	C7H16O	000589-82-2	9
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	9
4	PROPYLENE GLYCOL TRIMER 1	174	C9H18O3	000000-00-0	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

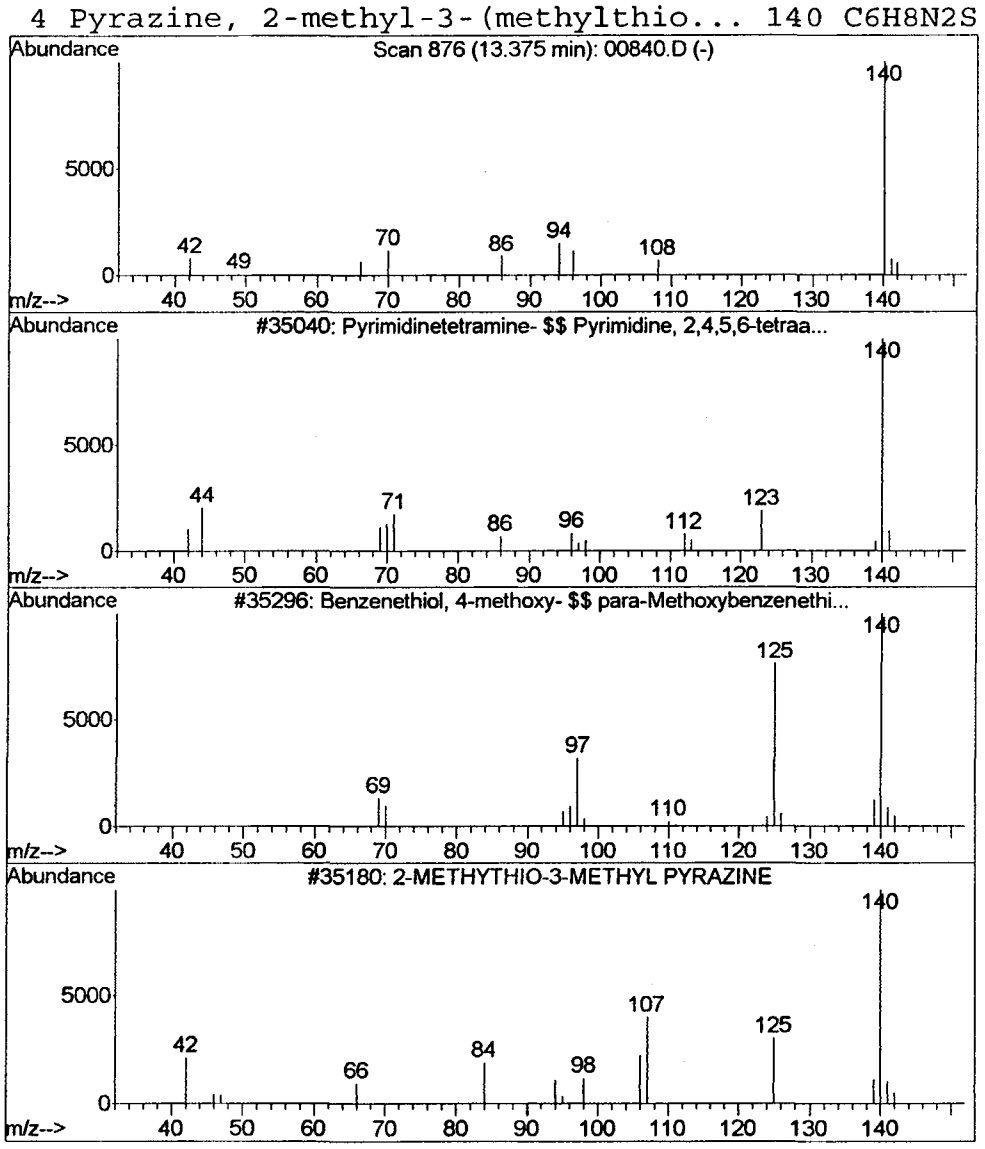
****

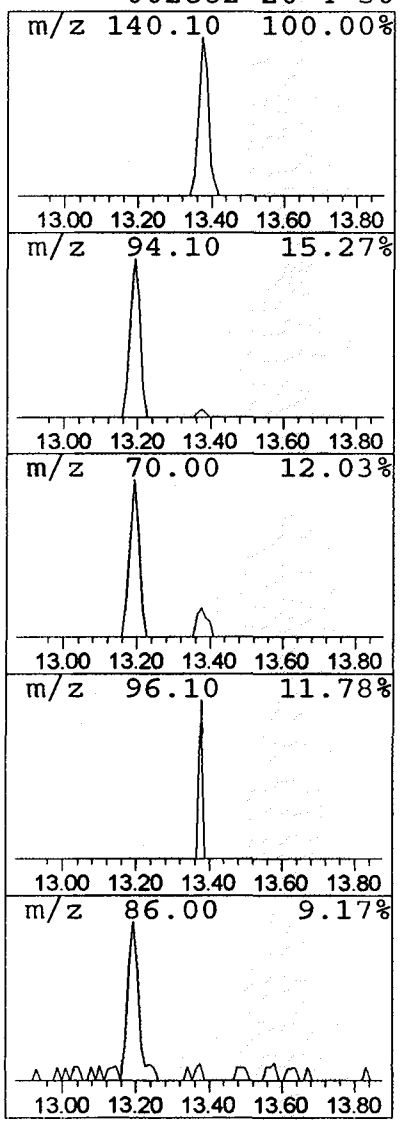
Peak Number 9 Pyrimidinetetramine- $$ Pyr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	0.05 ug/L	35578	Naphthalene-d8	13.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidinetetramine- $$ Pyrimidi...	140	C4H8N6	001004-74-6	64
2	Benzenethiol, 4-methoxy- $$ para...	140	C7H8OS	000696-63-9	64
3	2-METHYTHIO-3-METHYL PYRAZINE	140	C6H8N2S	002882-20-4	64
4	Pyrazine, 2-methyl-3-(methylthio...	140	C6H8N2S	002882-20-4	50

NO GOOD MATCH





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

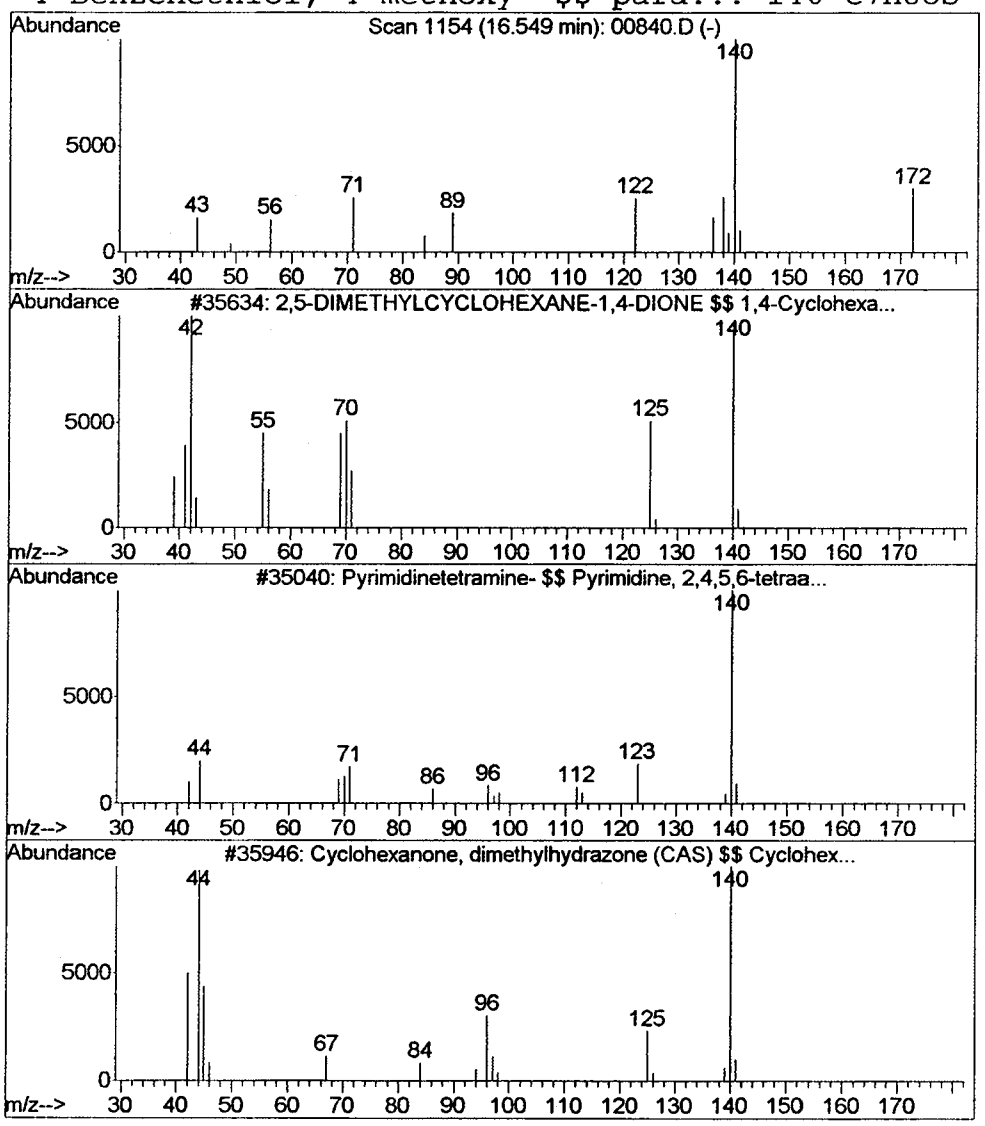
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

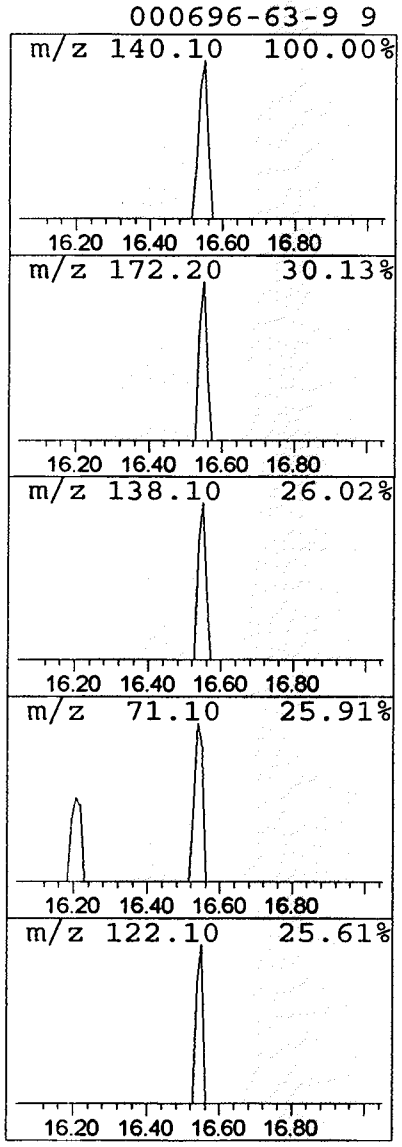
****

Peak Number 10 2,5-DIMETHYLCYCLOHEXANE-1,4... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	0.05 ug/L	35098	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-DIMETHYLCYCLOHEXANE-1,4-DION...	140	C8H12O2	000583-81-3	38
2	Pyrimidinetetramine- $$ Pyrimidi...	140	C4H8N6	001004-74-6	37
3	Cyclohexanone, dimethylhydrazone...	140	C8H16N2	010424-93-8	37
4	Benzenethiol, 4-methoxy- $$ para...	140	C7H8OS	000696-63-9	9





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

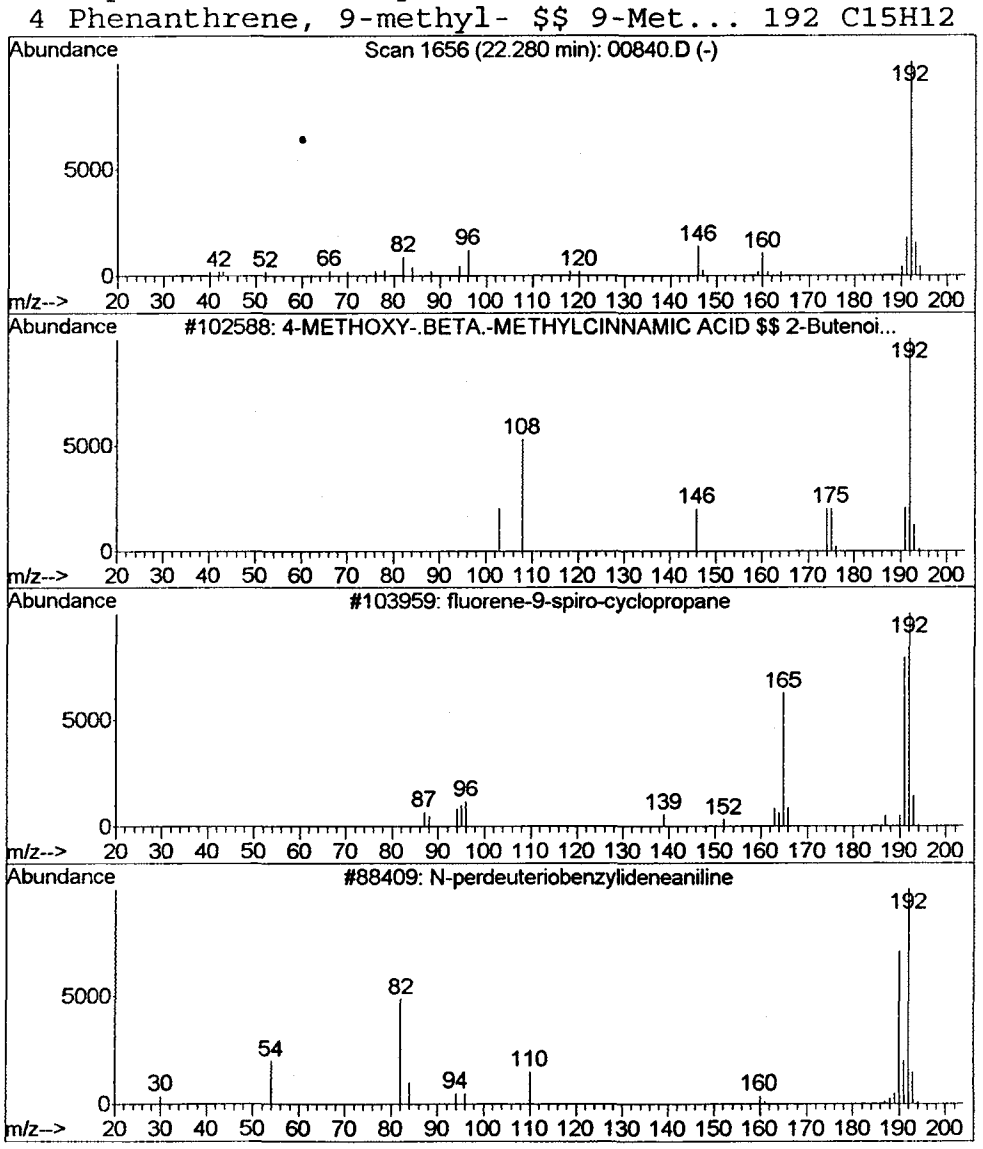
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

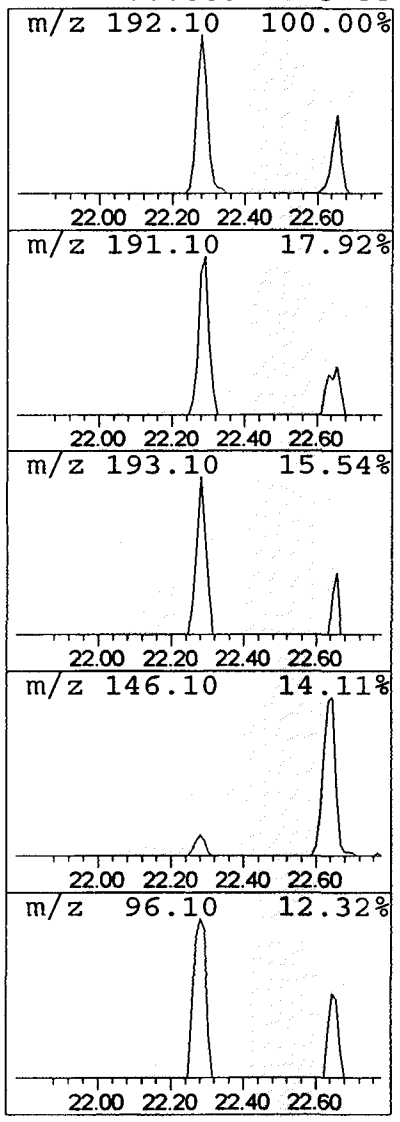
****

Peak Number 11 4-METHOXY-.BETA.-METHYLCINN... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.16 ug/L	124660	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-METHOXY-.BETA.-METHYLCINNAMIC ...	192	C11H12O3	019169-94-9	72
2	fluorene-9-spiro-cyclopropane	192	C15H12	000000-00-0	59
3	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	59
4	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	53





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

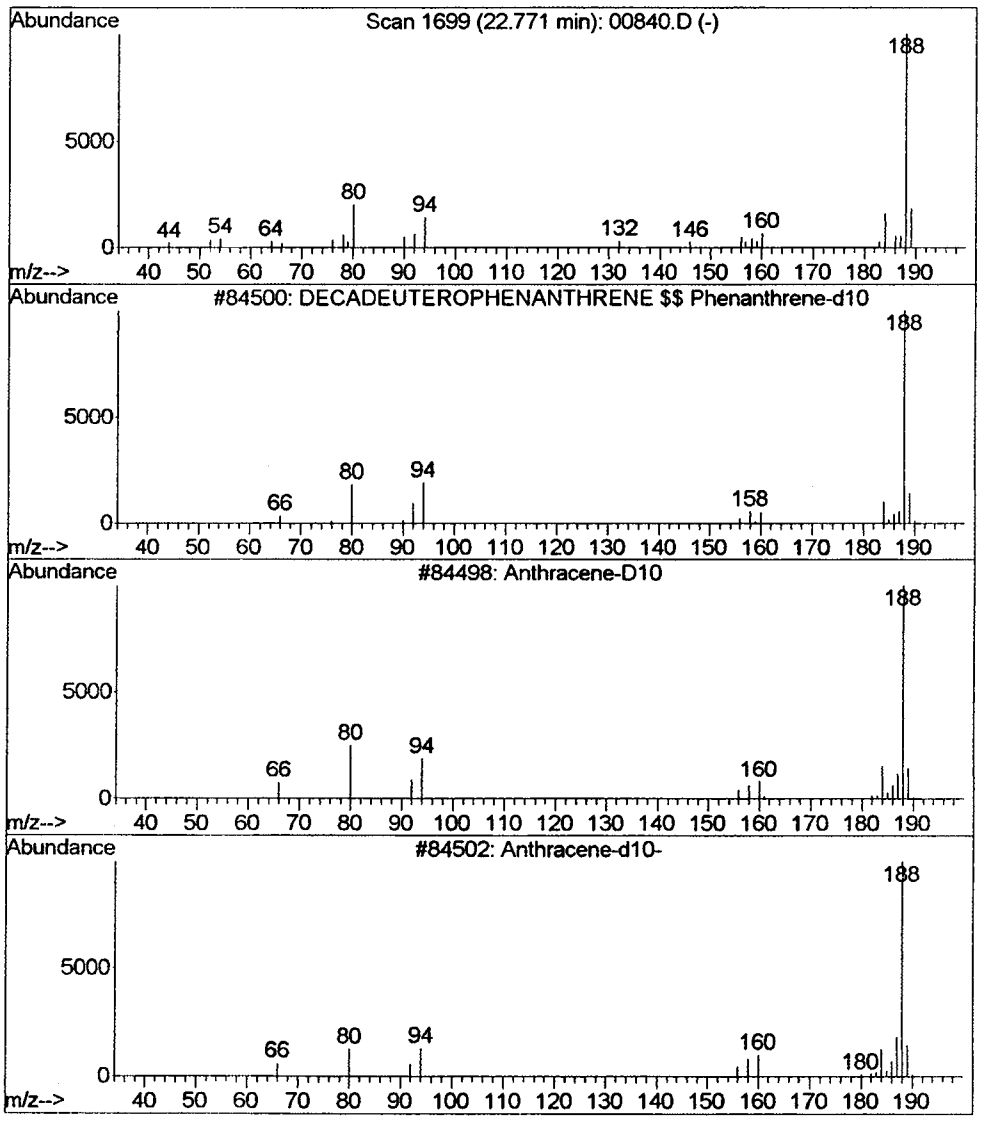
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

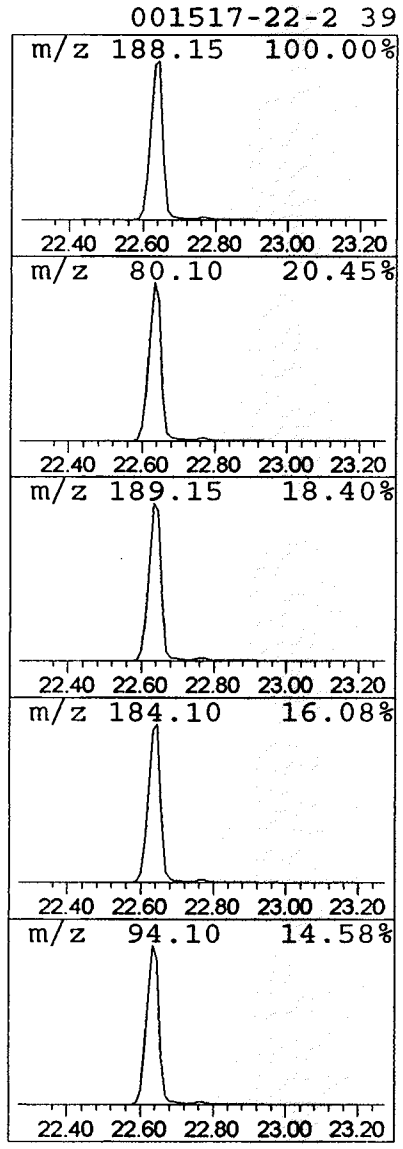
****

Peak Number 12 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.53 ug/L	416882	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	90
2	Anthracene-D10	188	C14D10	000000-00-0	87
3	Anthracene-d10-	188	C14D10	001719-06-8	72
4	Phenanthrene-d10	188	C14D10	001517-22-2	39





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00840.D Vial: 4
Acq On : 31 Jan 2002 5:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

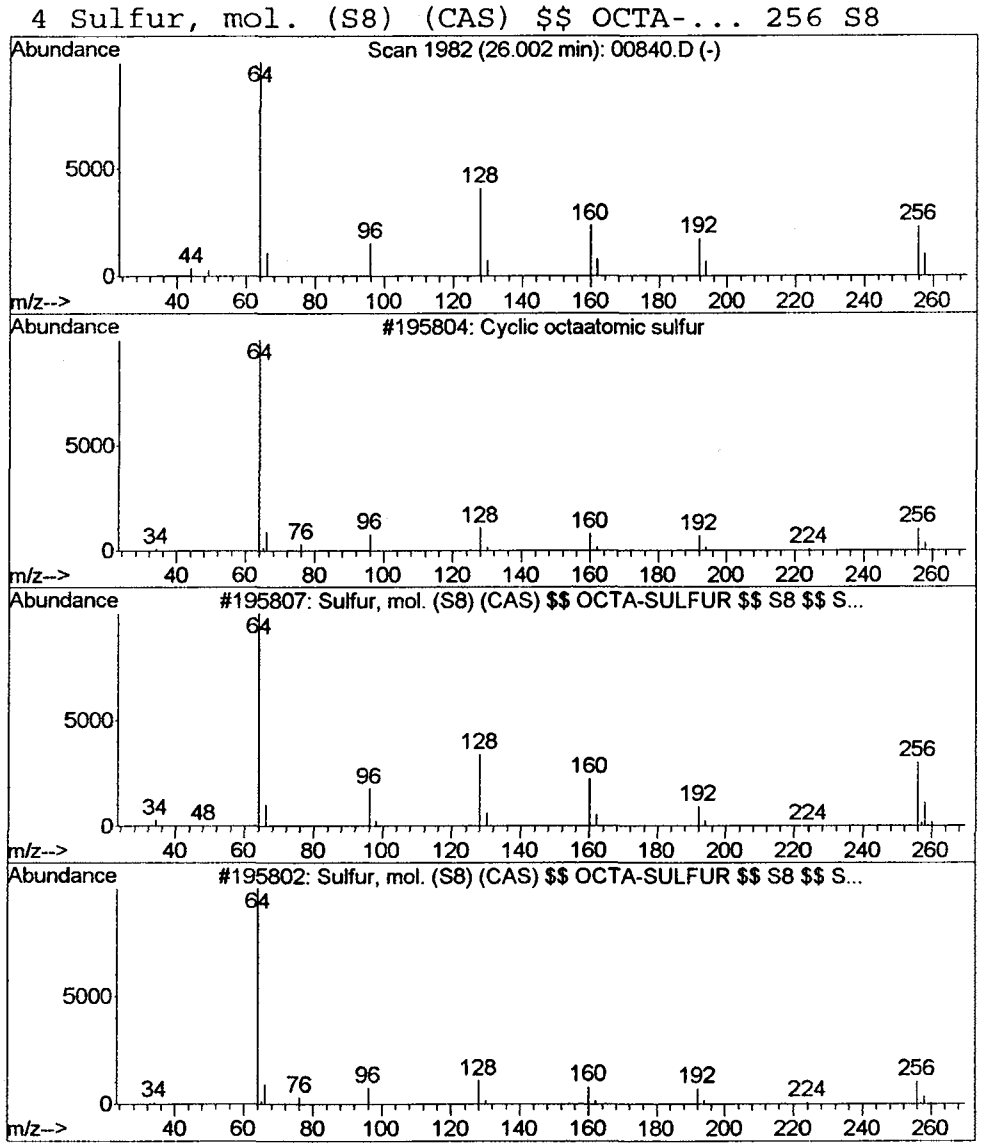
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

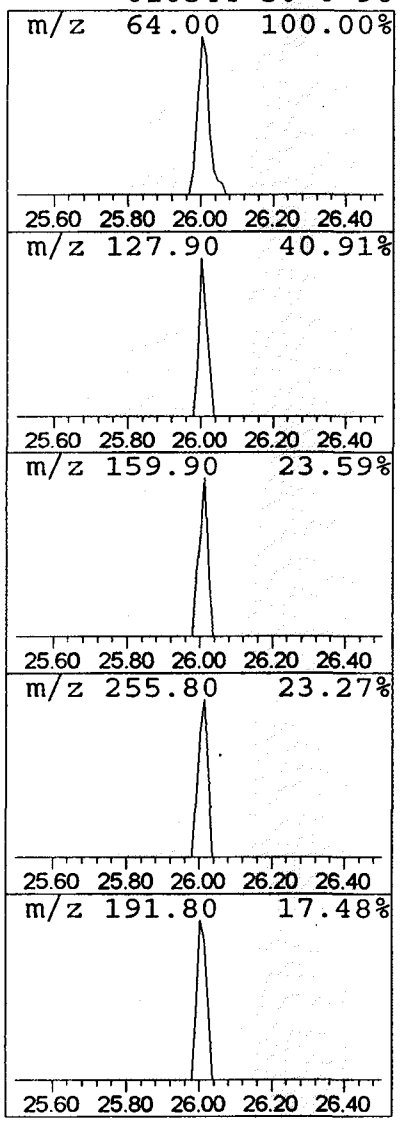
****

Peak Number 13 Cyclic octaatomic sulfur Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.00	0.05 ug/L	40579	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	91
2	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	91
3	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	91
4	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	90





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 31 Jan 2002 5:11 pm
Data File: C:\MSDCHEM\1\5973N\02JAN31\00840.D
Name: 508 scan
Misc: January 31, 2002
Method: C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title: 508 scan method
Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--- #	RT	Resp	Conc
Butanoic acid, me...	3.61	0.1	ug/L	52027	1	9.71	9625840	20.0
ISOBUTYRALDEHYDE...	3.92	0.1	ug/L	25435	1	9.71	9625840	20.0
1-Methylene-1,3-d...	4.25	0.1	ug/L	28414	1	9.71	9625840	20.0
Cyclobut-1-enylme...	4.87	0.1	ug/L	33762	1	9.71	9625840	20.0
3-Pentanol, 2,4-d...	5.92	0.4	ug/L	190779	1	9.71	9625840	20.0
2-Propanone, 1,1,...	6.00	0.1	ug/L	57741	1	9.71	9625840	20.0
1-(Dimethylamino)...	9.65	0.1	ug/L	39187	1	9.71	9625840	20.0
2-Propanol, 1-(2-...	9.86	0.1	ug/L	60202	1	9.71	9625840	20.0
Pyrimidinetetrami...	13.37	0.1	ug/L	35578	2	13.19	13772300	20.0
2,5-DIMETHYLCYCLO...	16.55	0.0	ug/L	35098	3	18.34	14679700	20.0
1-METHOXY-.BETA.-...	22.28	0.2	ug/L	124660	4	22.65	15867900	20.0
DECADEUTEROPHENAN...	22.77	0.5	ug/L	416882	4	22.65	15867900	20.0
Cyclic octaatomic...	26.00	0.1	ug/L	40579	4	22.65	15867900	20.0